

An exploration into the amide-pseudo amide hydrogen bonding synthon between a new coformer with two primary amide groups and theophylline†

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Electronic Supplementary Information

NMR Spectroscopy

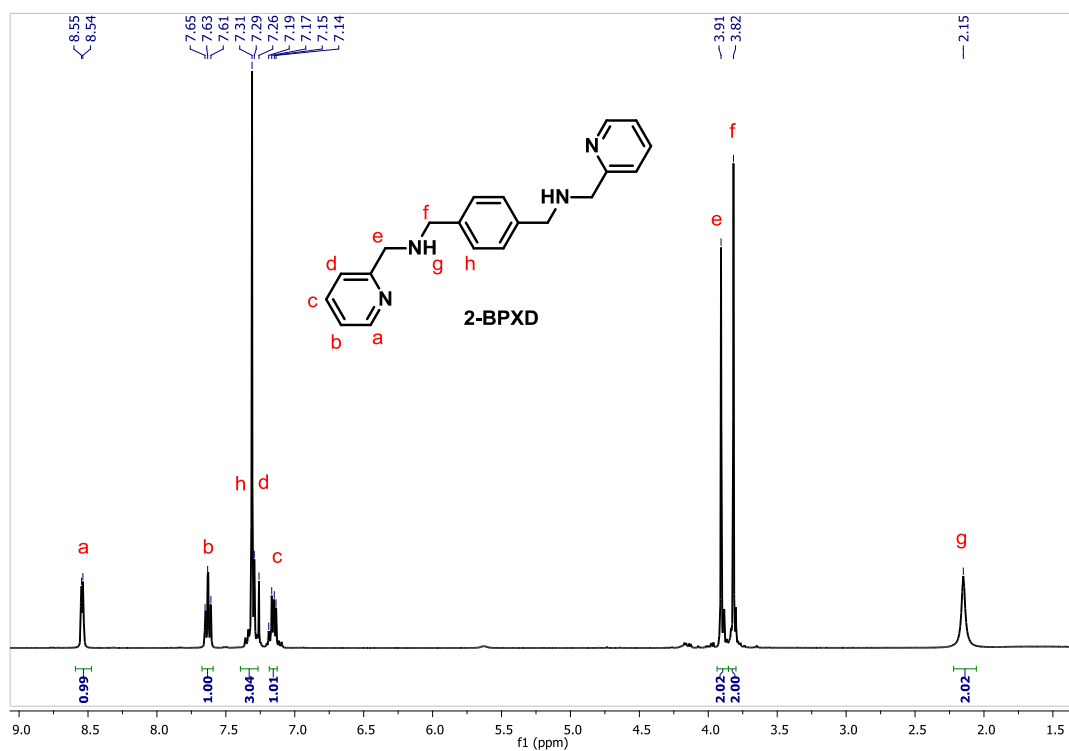


Fig. S1 ^1H NMR of step-1 (2-BPXD) in CDCl_3 .

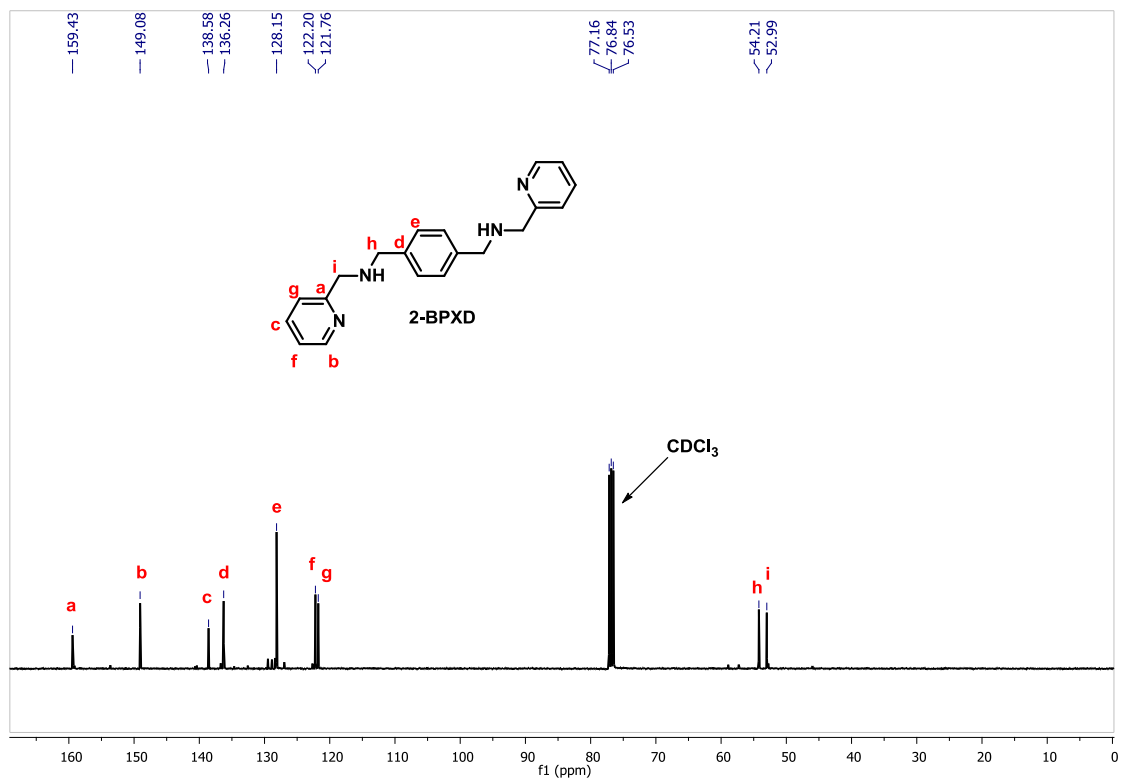


Fig. S2 ^{13}C NMR of step-1 (2-BPXD) in CDCl_3 .

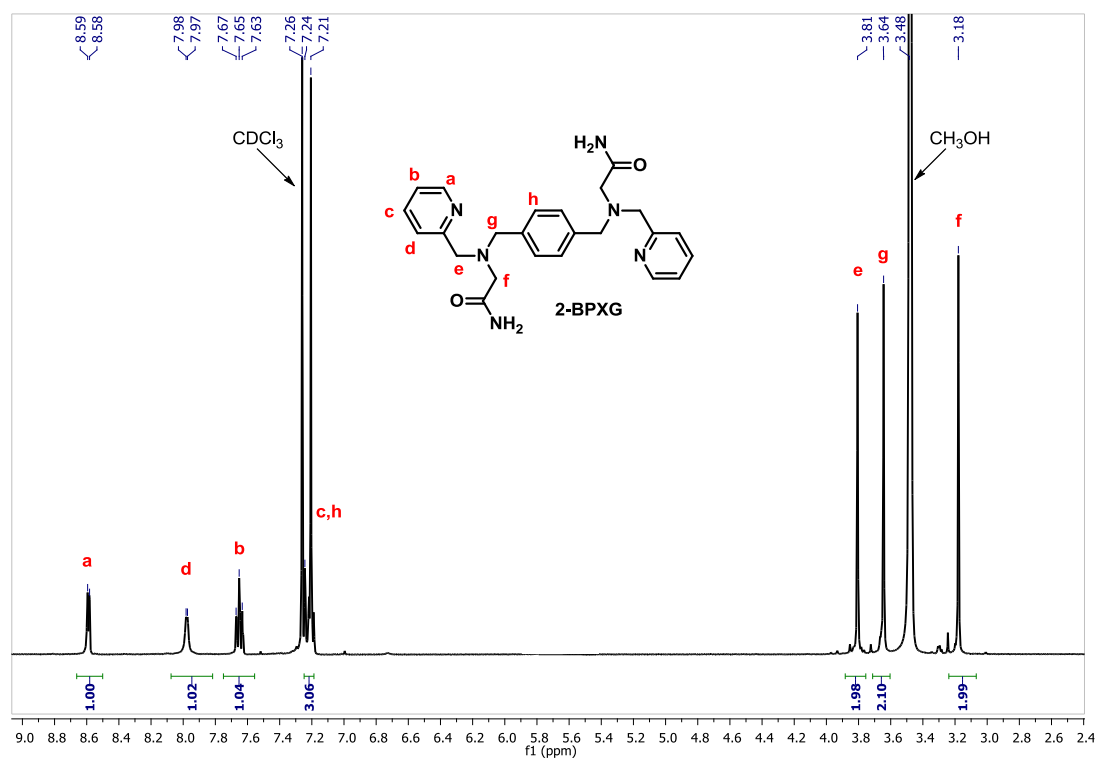


Fig. S3 ¹H NMR of step-2 (2-BPXG) in CDCl₃.

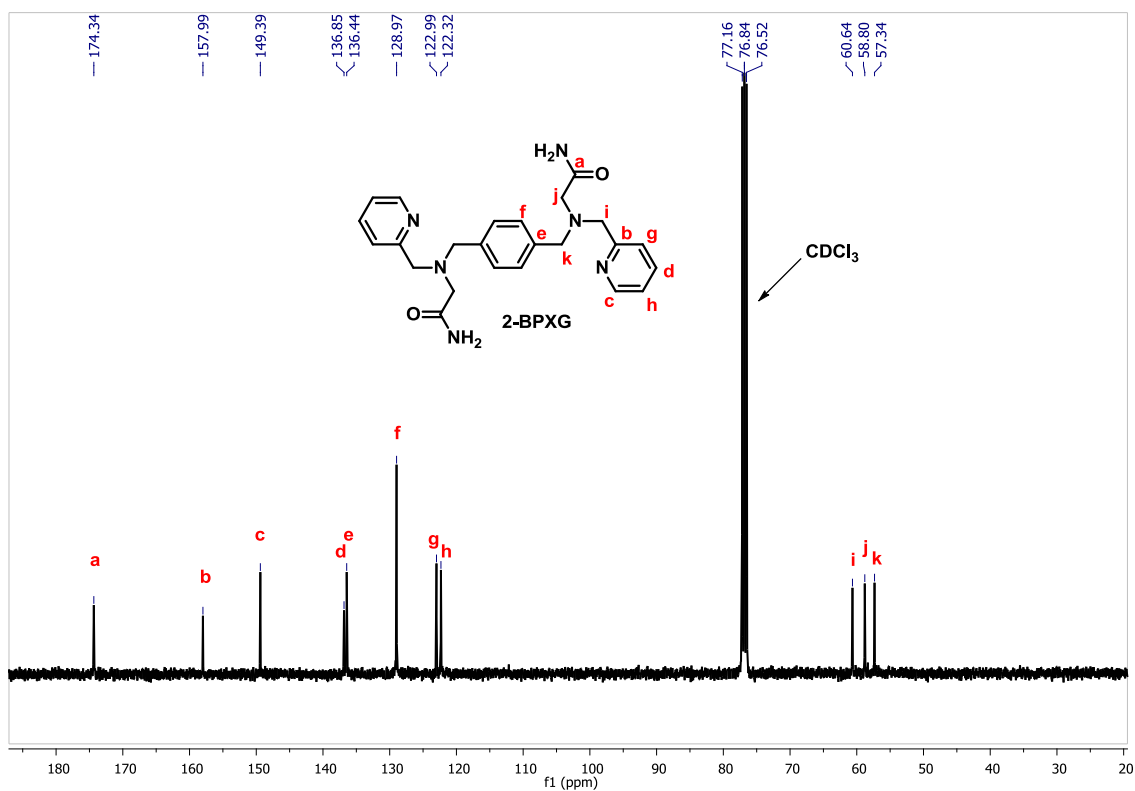


Fig. S4 ¹³C NMR of step-2 (2-BPXG) in CDCl₃.

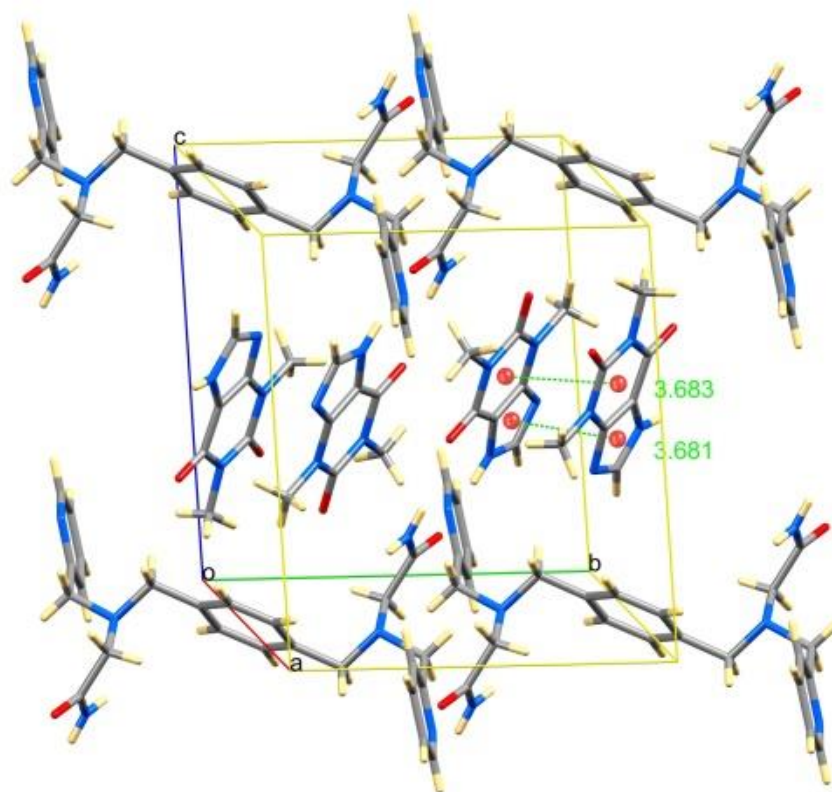


Fig. S5 Unit cell of **2-BPXG-4THP**, where strong π - π interactions between the **THP** molecules are indicated.

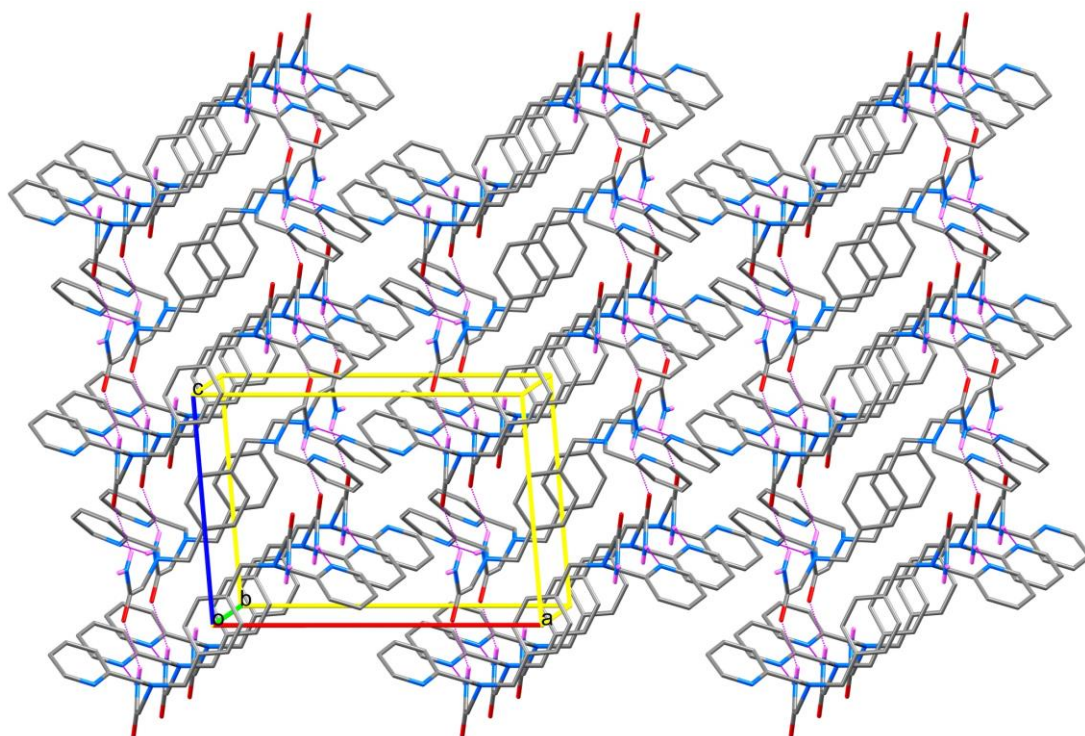


Fig. S6 Stacking of the 2D supramolecular network with its unit cell highlighted for **2-BPXG**.

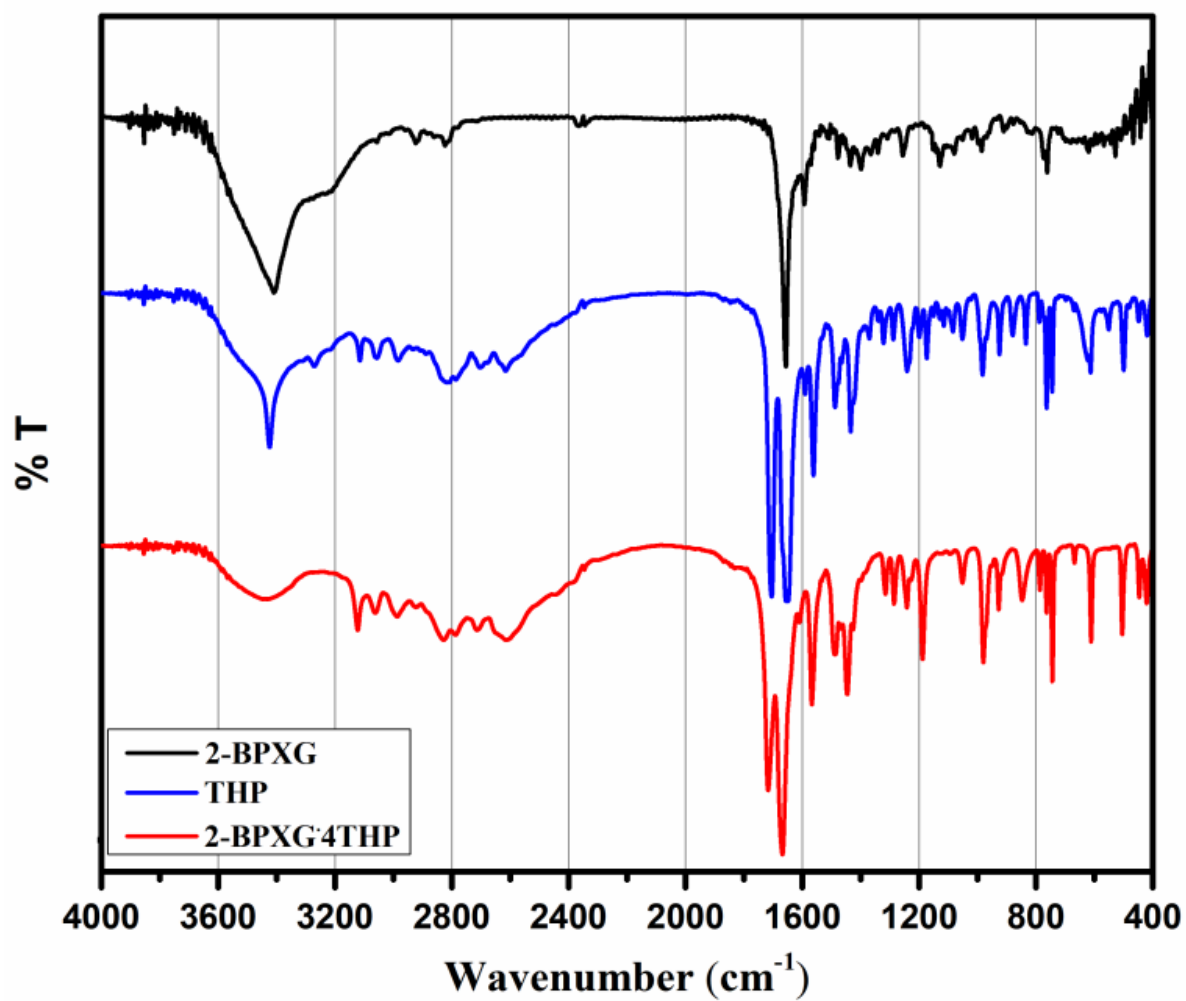


Fig. S6 FT-IR spectra of **2-BPXG**, **2-BPXG·4THP** and **THP** in the full region of 400–4000 cm⁻¹.

Differential Scanning Calorimetry (DSC)

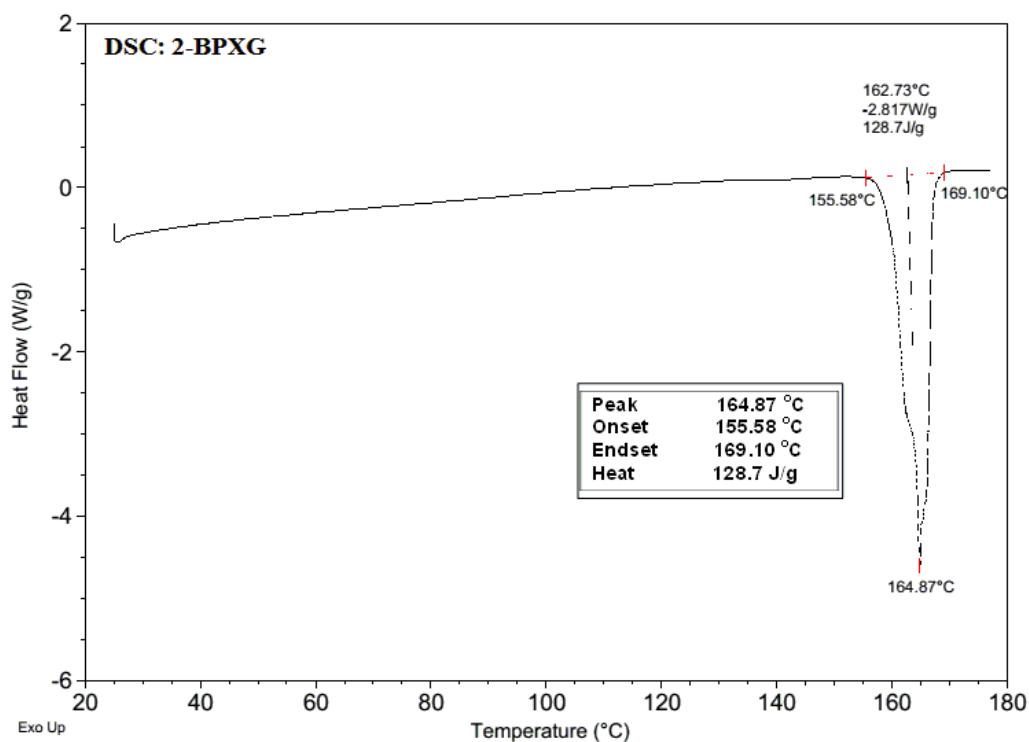


Fig. S8 DSC curve of a 2-BPXG recorded at a 10 °C min⁻¹ heating rate.

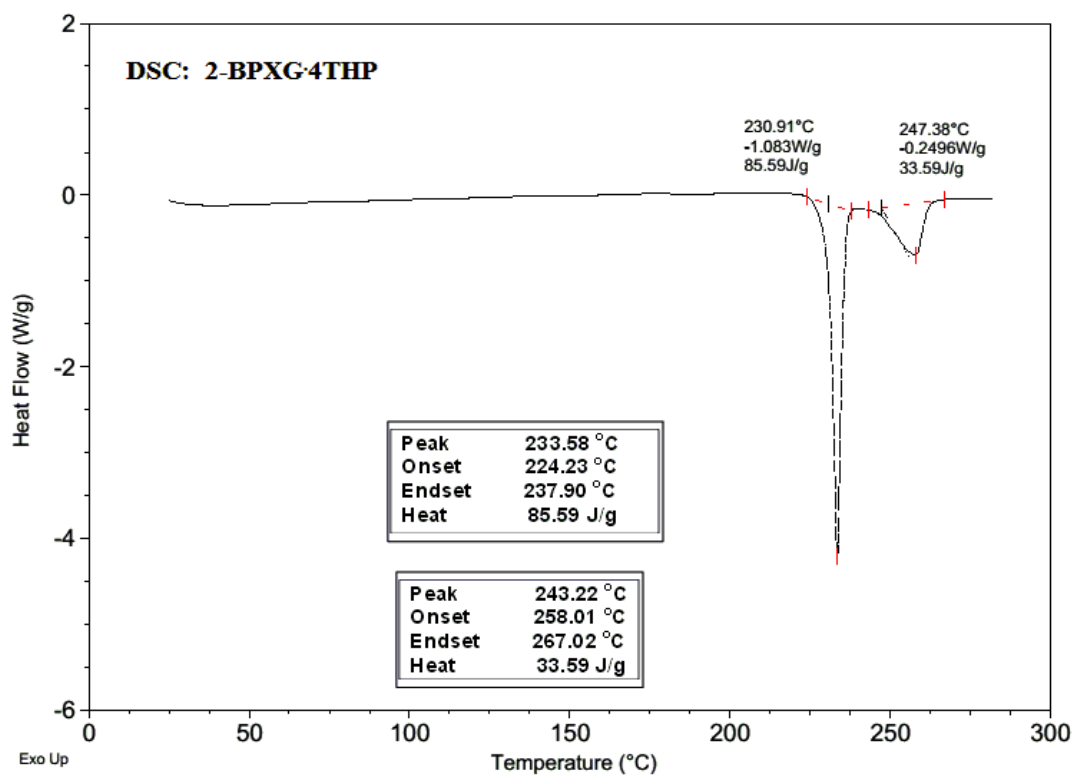


Fig. S9 DSC curve of a 2-BPXG·4THP recorded at a 10 °C min⁻¹ heating rate.